Acta Cryst. (1964). **17**, 762

Structural relationships in beryllium-titanium alloys.

By E. Gillam* and H. P. Rooksby, *The General Electric Company Limited, Central Research Laboratories, Hirst Research Centre, Wembley, England* and L. D. Brownlee, *Associated Electrical Industries Limited, Research Laboratories, Trafford Park, Manchester, England*

(*Received* 15 *November* 1963)

Some years ago Raeuchle & Rundle (1952) described the structure of $Be_{12}Ti$ as disordered hexagonal, with $a_0 = 29{\cdot}44$ and $c_0 = 7{\cdot}33$ Å, from an X-ray study of a single crystal. More recently, Zalkin, Sands, Bedford & Krikonian (1961) have reported a tetragonal structure for this phase, the analysis being made from powder patterns.

During investigations of alloys of beryllium carried out by the present authors, also by powder methods, beryllium-rich alloys of beryllium and titanium have consistently shown the presence of a constituent of tetragonal structure similar to that of Zalkin. It was also noticed that the alloy $Be_{12}V$ gave a very similar powder pattern, indicative of an isostructural character. The literature data and those obtained in the work reported here are compiled in Table 1.

Table 1 also includes structure data which have been reported for another Be–Ti phase of composition $Be_{17}Ti_2$. Although these data differ somewhat in detail, it is clear from a glance at the figures that they are all based on a similar primitive cell of hexagonal symmetry. Moreover it is possible to deduce a relationship with the tetragonal structure of $Be_{12}Ti$.

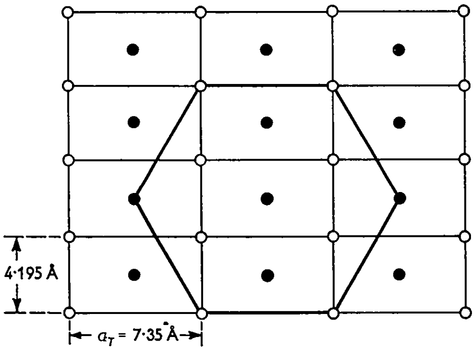

Fig. 1. Hexagonal cell derived from Be_{12} Ti tetragonal cells with $a_T/c_T = \sqrt{3}$.

○ Ti atoms at $a=0$ level
● Ti atoms at $a=\frac{1}{2}$ level
Be atoms not shown.

By analogy with the structure of $Be_{12}V$ (and also that of $Be_{12}Cr$) we are justified in assuming that tetragonal $Be_{12}Ti$ has the *A*6 $Mn_{12}Th$ structure, space group I_4/mmm. The relationship between this and the hexagonal $Be_{17}Ti_2$ structure then becomes apparent by reference to Fig. 1. Since for the tetragonal cell, a_T/c_T is very nearly equal to $\sqrt{3}$, a basic geometrically hexagonal cell can be outlined (shown by thick lines), for which $a_H = 7{\cdot}35$ Å and c_H = any multiple of 7·35 Å. The $[010]_T$ direction corresponds to the $[0001]_H$ direction.

Fig. 2 shows a projection on (010) of Mn atoms in the $Mn_{12}Th$ structure and this indicates how they (≡Be atoms in $Be_{12}Ti$) are arranged in near-hexagonal symmetry.

The series of alloys which we examined and which are mentioned in Table 1 gave X-ray powder patterns which were remarkably alike. The principal strong reflexions occurred at almost the same Bragg angles. The significant difference between the pattern of alloy IV, containing the hexagonal phase, and the others, lay chiefly in the manner in which some of the strong lines were split.

It appears probable therefore that the transition in structure with change of composition from $Be_{12}Ti$ to

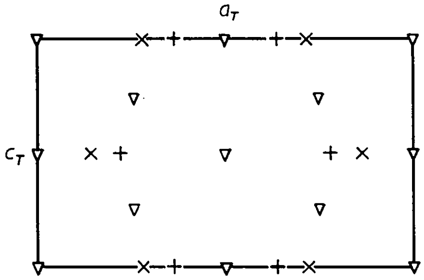

Fig. 2. Projection on (010) of Mn atoms in the $Mn_{12}Th$ structure

+	Mn atoms at $a=0$ level.	4 per unit cell
×	Mn atoms at $a=\frac{1}{2}$ level.	4 per unit cell
∇	Mn atoms at $a=0{\cdot}25$, 0·277, or 0·361 levels.	16 per unit cell

Table 1. *Structure data for beryllium alloys*

Alloy compositions used in I, II, III, and IV were respectively 1·5, 5·0, 20·0 and 31·0 wt.% Ti in Be.

Source	Phase	Lattice type and parameters			
Raeuchle & Rundle	$Be_{12}Ti$	Hexagonal	$a=29{\cdot}44$ Å	$c=7{\cdot}33$ Å	
Zalkin *et al.*	$Be_{12}Ti$	Tetragonal	$a=7{\cdot}35$	$c=4{\cdot}19$	
Present work I	$Be_{12}Ti$	Tetragonal	$a=7{\cdot}27$	$c=4{\cdot}195$	
Present work II	$Be_{12}Ti$	Tetragonal	$a=7{\cdot}36$	$c=4{\cdot}195$	
Present work III	$Be_{12}Ti$	Tetragonal	$a=7{\cdot}36$	$c=4{\cdot}195$	
Present work	$Be_{12}V$	Tetragonal	$a=7{\cdot}35$	$c=4{\cdot}24$	
Zalkin *et al.*	α-$Be_{17}Ti_2$	Rhombohedral	$a=7{\cdot}392$	$c=10{\cdot}79$	(Hex. axes)
Zalkin *et al.*	β-$Be_{17}Ti_2$	Rhombohedral	$a=7{\cdot}392$	$c=7{\cdot}30$	(Hex. axes)
Paine & Carrabine	$Be_{17}Ti_2$	Hexagonal	$a=7{\cdot}34$	$c=10{\cdot}73$	
Vainshtein, Blokhin & Kripyakevich (1962)	$Be_{17}Ti_2$	Trigonal	$a=7{\cdot}40$	$c=10{\cdot}84$	
Present work IV	$Be_{17}Ti_2$	Hexagonal	$a=7{\cdot}35$	$c=7{\cdot}26$	

---

* Now at The Sir John Cass College, London, E.C. 3, England.

β-$Be_{17}Ti_2$ is a relatively simple one, in which the $[010]_T$ direction becomes the $[0001]_H$ direction. Some titanium atoms must change from $a=0$ to $a=\frac{1}{2}$ positions, or *vice versa*, to complete the symmetry, and the removal of 7 Be atoms from the unit cell involves a small decrease in the atomic spacing in this direction, from 7·36 to about 7·30 Å. The removal of 7 atoms without disrupting the near-hexagonal symmetry displayed by the tetragonal arrangement in Fig. 2 appears difficult to accomplish. Removal of the two smaller layers is simple but results in a loss of 8 Be atoms. This raises the question of how accurately the composition of $Be_{17}Ti_2$ is known and whether a composition Be_8Ti is possible.

The other two hexagonal structures of Table 1 can be derived from this transformation. Raeuchle & Rundle's disordered hexagonal structure has the same c parameter as the β-$Be_{17}Ti_2$ structure and four times the a parameter; the α-$Be_{17}Ti_2$ structure has the same a parameter and approximately 1·5 times the c parameter. The above discussion also suggests the possibility that Raeuchle & Rundle's structure determination was carried out on crystals of $Be_{17}Ti_2$ instead of on crystals of $Be_{12}Ti$ as they believed.

References

Paine, R. M. & Carrabine, J. A. (1960). *Acta Cryst.* **13**, 680.

Raeuchle, R. F. & Rundle, R. E. (1952). *Acta Cryst.* **5**, 85.

Vainshtein, E. E., Blokhin, S. M. & Kripyakevich, P. I. (1962). *Doklady Akad. Nauk SSSR*, **142**, 85.

Zalkin, A., Sands, D. E., Bedford, R. G. & Krikonian, O. H. (1961). *Acta Cryst.* **14**, 63.

Acta Cryst. (1964). **17**, 763

Direct high-temperature single-crystal observation of orientation relationship in zirconia phase transformation.

By G. M. Wolten, *Aerospace Corporation, El Segundo, California, U.S.A.*

(*Received* 7 *October* 1963 *and in revised form* 24 *October* 1963)

Introduction

Zirconia undergoes a diffusionless phase transformation, in the neighborhood of 1000 °C, from a monoclinic structure, space group $P2_1/c$, to a tetragonal structure, space group $P4_2/nmc$.

From the data of McCullough & Trueblood (1959) for monoclinic zirconia and those of Teufer (1962) for tetragonal zirconia, one can draw the two projections of the structures shown in Figs. 1 and 2. The projections show four unit cells of the monoclinic structure. A fifth cell, indicated by dashed lines, differs only by the choice of origin in order to render it more directly comparable to the single tetragonal unit cell shown to the right. The tetragonal cell shown is not the conventional cell, but a double one that traditionally has been used for comparison

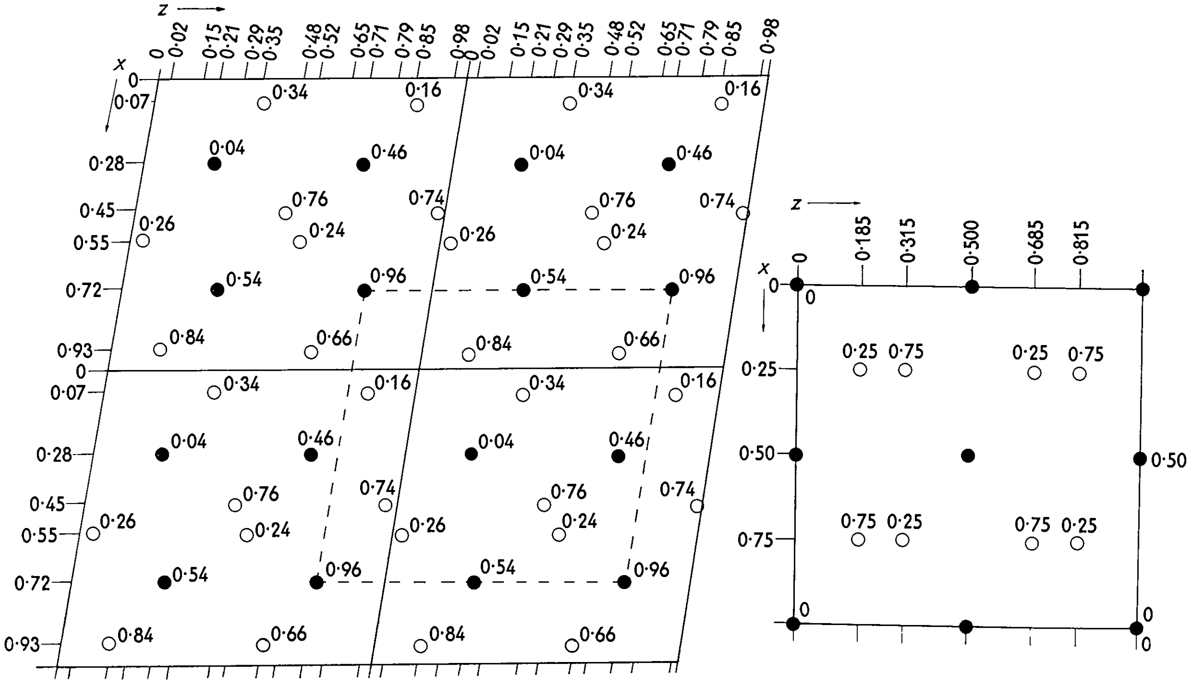

Fig. 1. Projection of ZrO_2 structure parallel to y direction onto x–z plane. Left: monoclinic. Right: Tetragonal. Parts of four monoclinic cells enclosed by broken lines become tetragonal cell after transformation. Solid circles: Zr. Open circles: O.